

Supersolidity in the triangular lattice spin-1/2 XXZ model: A variational perspective

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We study the spin-1/2 XXZ model on the triangular lattice with a nearest neighbor antiferromagnetic Ising coupling $J_z > 0$ and unfrustrated ($J_\perp < 0$) or frustrated ($J_\perp > 0$) kinetic terms in zero magnetic field. Incorporating long-range Jastrow correlations over a mean field spin state, we obtain the variational phase diagram of this model on large lattices for arbitrary J_z and either sign of J_\perp . For $J_\perp < 0$, we find a $\sqrt{3} \times \sqrt{3}$ supersolid for $J_z/|J_\perp| \gtrsim 4.7$, in excellent agreement with quantum Monte Carlo data. For $J_\perp > 0$, a distinct $\sqrt{3} \times \sqrt{3}$ supersolid is found to emerge for $J_z/J_\perp \geq 1$. Both supersolids exhibit a spontaneous density deviation from half-filling. At $J_z/J_\perp = \infty$, the crystalline order parameters of these two supersolids are nearly identical, consistent with exact results.

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Introduction. — Understanding how quantum effects select a unique ground state from an exponentially large number of classically degenerate configurations is a problem that is common to geometrically frustrated magnets, Mott insulators, and quantum Hall systems. The simplest example of a frustrated classical magnet is the two-dimensional (2D) classical Ising antiferromagnet on the triangular lattice, which has an extensive ground state entropy, with an entropy per spin ≈ 0.323 , and critical $\sqrt{3} \times \sqrt{3}$ spin correlations [1]. The application of an infinitesimal transverse magnetic field is known to lift this ground state degeneracy and favor a long-range $\sqrt{3} \times \sqrt{3}$ ordered state [2] where the sublattice magnetizations on the three sublattices take on the form $(0, m_z, -m_z)$. Another quantum variant is the triangular lattice spin-1/2 XXZ model, described by the Hamiltonian

$$H = \sum_{\langle ij \rangle} [J_z S_i^z S_j^z + J_\perp (S_i^x S_j^x + S_i^y S_j^y)], \quad (1)$$

where $J_z > 0$ and $\langle ij \rangle$ refer to nearest neighbour links of the triangular lattice; interest in this model stems from an early suggestion [3] that this model might support, for $J_\perp > 0$, a quantum spin liquid ground state for $J_z/J_\perp \gg 1$. (Henceforth, we will set $|J_\perp| = 1$.) This model may also be viewed as a hard-core boson model with a nearest neighbor boson repulsion and a boson hopping amplitude which is unfrustrated ($J_\perp < 0$) or frustrated ($J_\perp > 0$). Interest in such models has been revived following reports [4] of supersolidity in ^4He which remain to be understood.

In this paper, using a variational wave function which incorporates long range Jastrow correlations, together with recently developed Monte Carlo optimization methods [5], we obtain the variational phase diagram of this model on large lattice sizes for either sign of J_\perp . The main significance of our work, apart from the fact that it represents substantial progress in the study of the XXZ model, is that it illustrates the power of the variational wave function approach in studying strongly correlated phases and quantum phase transitions.

We begin by summarizing our key results in the context of recent important work on this model.

For $J_\perp < 0$: (i) We incorporate Jastrow correlations above a uniform superfluid wave function and find, using the Binder cumulant, a phase transition from a correlated superfluid state into a supersolid with long range $\sqrt{3} \times \sqrt{3}$ crystal order for $J_z \gtrsim 4.7$; this supersolid order persists even for $J_z \rightarrow \infty$. This is in good agreement with quantum Monte Carlo (QMC) simulation results [8–10] which found a superfluid-supersolid transition at $J_z \approx 4.5$. (ii) We find that the Jastrow factors exhibit a long range $1/r$ tail in the superfluid as well as the supersolid which is consistent with a linearly dispersing sound mode. (iii) The crystal order in the supersolid emerges as a *spontaneously* broken symmetry in our wave function as a consequence of Jastrow correlations, but the Jastrow factors do not completely fix the crystal pattern. Incorporating a variational parameter which directly couples to the difference between the $(2m_z, -m_z, -m_z)$ and $(0, m_z, -m_z)$ candidate crystal orders, we find that the former has a slightly lower energy, consistent with QMC results [8, 10, 11] as well as a recent variational study [12] of the quantum dimer model at $J_z = \infty$. (iv) We find that a supersolid wave function which permits for a small density deviation away from half-filling has lower energy.

For $J_\perp > 0$: (i) We incorporate Jastrow correlations on top of a state with coplanar 3-sublattice magnetic order. Using this wave function, we find that there is 120° -xy order for $J_z < 1$ whereas there is supersolid order for $J_z \gtrsim 1$, with $(2m_z, -m_z, -m_z)$ crystal order, in agreement with a recent suggestion based on analyzing the $J_z = \infty$ limit [6] and density matrix renormalization group (DMRG) results on small system sizes [7]. (ii) The formation of the supersolid state is accompanied by a spontaneous density deviation away from half-filling. Equivalently, the XXZ model in zero field develops a spontaneous S^z magnetization; this magnetization grows with increasing J_z . (iii) The 120° -xy state as well as the supersolid exhibit $1/r$ decay of Jastrow factors consistent with a linearly dis-

persing excitation mode. (iv) For $J_z = \infty$, recent work has shown, through the construction of a unitary transformation [6] as well as by a high temperature expansion [7], that the diagonal spin correlations are identical for either sign of J_\perp in this limit, which enables one to conclude that the frustrated XXZ model must also exhibit $\sqrt{3} \times \sqrt{3}$ crystal order, and is likely to be a supersolid at $J_z = \infty$ [6, 7]. At $J_z = \infty$, the crystal orders in our ‘frustrated supersolid’ and the ‘unfrustrated supersolid’ are nearly identical and close to QMC results for $J_\perp < 0$, in agreement with this result. (v) In contrast to the result of Ref. [6], we find that the off-diagonal order parameter for $J_\perp > 0$ is much smaller than that for $J_\perp < 0$.

Variational Wave function. — We begin with a variational wave function of the form

$$|\psi_V\rangle = \mathcal{J}_\theta \exp\left(\sum_{i,\mathbf{r}} \mathcal{J}(\mathbf{r}) S_i^z S_{i+\mathbf{r}}^z\right) \mathcal{P}_G |\psi_{\text{MF}}\rangle, \quad (2)$$

where $|\psi_{\text{MF}}\rangle$ is a variational mean-field wave function for spin- \uparrow and spin- \downarrow fermions (see below), \mathcal{P}_G is the Gutzwiller projection operator which restricts the Hilbert space to one fermion per site thus taking us from a fermionic state to a spin wave function, $\mathcal{J}(\mathbf{r})$ are variational Jastrow parameters which build correlations between spins separated by \mathbf{r} while respecting lattice symmetries, and \mathcal{J}_θ is a global variational parameter, elaborated upon later, which fully fixes the crystalline order.

We choose $|\psi_{\text{MF}}\rangle$ to be the ground state of a mean field Hamiltonian $H_{\text{MF}} = -\sum_{\langle ij \rangle} t_{ij}^{\text{var}} c_{i\sigma}^\dagger c_{j\sigma} - \sum_i \vec{h}_i^{\text{var}} \cdot \vec{S}_i$, where $\vec{S}_i = \frac{1}{2} c_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{i\beta}$. The first term in H_{MF} represents nearest neighbor hopping of fermions, with amplitudes t_{ij}^{var} , while the second term represents a site-dependent magnetic field whose direction and magnitude can be chosen to yield various magnetically ordered states. Note that the wave function has the freedom to describe a magnetically disordered spin liquid state if $h_i^{\text{var}} = 0$.

For the unfrustrated model ($J_\perp = -1$) we set $t_{ij}^{\text{var}} = 0$, and select two different configurations of \vec{h}_i^{var} . One choice is to set $\vec{h}_i^{\text{var}} = \hat{x}$, which leads to a mean field ferromagnet with the moment polarized along the S^x direction. This mean field state has no variational parameters; we refer to the spin wave function, after Gutzwiller projecting this state and inclusion of correlation factors, as $|\Psi_V^{\text{FM-x}}\rangle$. The second choice, which we motivate below, promotes 3-sublattice magnetic order, with $h_{i,z}^{\text{var}} = (1, -1/2, -1/2)$ on the 3 sublattices, $h_{i,x}^{\text{var}} = h_x$, and $h_{i,y}^{\text{var}} = 0$, where h_x is a variational parameter. We refer to the correlated spin state obtained from this mean field state as $|\Psi_V^{\text{FM-xz}}\rangle$.

For the frustrated model, we choose the hopping amplitudes such that $|t_{ij}^{\text{var}}| = 1$ but with signs picked such that upward (downward) pointing triangular plaquettes enclose flux π (zero). Upon Gutzwiller projection, this state describes a spin liquid which preserves all lattice symmetries. It is equivalent to a pairing wave function which is known, from earlier studies [5] to be a good start-

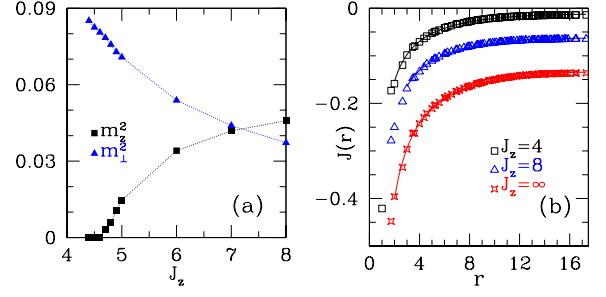


FIG. 1: (Color online) (a) Order parameters, extrapolated to the thermodynamic limit, for $J_\perp = -1$. (b) Jastrow parameters showing $1/r$ behavior at long distance (curves for $J_z = 4, \infty$ have been offset downward for clarity).

ing point to understand the triangular Heisenberg antiferromagnet. Motivated by the classical ground state, we pick \vec{h}_i^{var} to describe 3-sublattice coplanar magnetic order. The spin wave function obtained from choosing $h_{ix}^{\text{var}} = (h, -h/2, -h/2)$, $h_{iy}^{\text{var}} = (0, h\sqrt{3}/2, -h\sqrt{3}/2)$, and $h_{iz}^{\text{var}} = 0$, with h being a mean field variational parameter, will be called $|\Psi_V^{\text{AF-xy}}\rangle$. The spin wave function obtained from choosing $h_{ix}^{\text{var}} = (0, h_x, -h_x)$, $h_{iy}^{\text{var}} = (h_z, -h_z/2, -h_z/2)$, and $h_{iz}^{\text{var}} = 0$, with mean field variational parameters h_x, h_z , will be called $|\Psi_V^{\text{AF-xz}}\rangle$.

In order to obtain the best trial wave function, we optimize the variational parameters using Monte Carlo sampling of the spin configurations combined with recently developed techniques [5]. We begin by discussing our results for the unfrustrated model, for which we present comparisons with existing QMC results. We follow it up with results on the frustrated model which is less well studied since the sign problem does not permit controlled QMC simulations. Finally, we consider $J_z = \infty$, and demonstrate consistency with exact results in this limit.

$J_\perp < 0$, Unfrustrated Case. — For $J_z \ll 1$, the ground state of the unfrustrated model is a quantum ferromagnet or, equivalently, a superfluid state of hard core bosons. With increasing J_z , the ground state of the superfluid becomes increasingly correlated, and QMC simulations [8–11] show that a supersolid ground state, with coexisting superfluid and charge order, develops for $J_z \gtrsim 4.5$. If we set $\mathcal{J}_\theta = 1$ and optimize $|\Psi_V^{\text{FM-x}}\rangle$, we find that the ferromagnetic order parameter $m_1^2 = |\langle S^x \rangle|^2$ is nonzero for all values of J_z , as seen from Fig. 1(a), consistent with superfluidity persisting for arbitrarily large interactions. For all interaction strengths, we also find, as seen from Fig. 1(b), that the optimal Jastrow parameters $\mathcal{J}(\mathbf{r})$ decay as $1/r$ with distance. Such a power law decay implies a density structure factor scaling as $\sim |\mathbf{q}|$ at small momenta which is consistent with a linearly dispersing Goldstone mode above a superfluid ground state [13]. It is a nontrivial test of the unbiased variational optimization that we recover this behavior by optimizing over a very large set of variational Jastrow parameters.

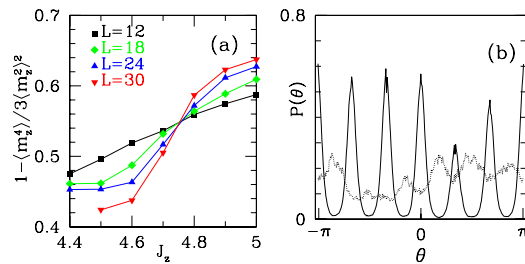


FIG. 2: (Color online) (a) Binder cumulant crossing for m_z displaying a superfluid-supersolid transition at $J_z^{(\text{crit})} \approx 4.7$. (b) Probability distribution of the phase of order parameter for $h_\theta = 0$ (dashed line) and at the optimal $h_\theta > 0$ (solid line).

In order to probe for supersolidity, we compute the density structure factor (equivalently S^z correlations). Although $|\Psi_V^{\text{FM-x}}\rangle$ is a translationally invariant state, we find that the density structure factor diverges at momenta $\pm(4\pi/3, 0)$ for large J_z which shows that there is $\sqrt{3} \times \sqrt{3}$ crystalline ordering, that coexists with the superfluidity, for strong interactions. It is remarkable that the crystalline order emerges as a *spontaneously broken symmetry* induced by Jastrow correlations in our wave function. Using the crossing of the Binder cumulant on different system sizes as shown in Fig. 2(a), as well as from a calculation of the order parameters extrapolated to infinite system sizes shown in Fig. 1(a), we locate the superfluid to supersolid transition point at $J_z^{(\text{crit})} \approx 4.7$, which is in good agreement with QMC simulation results.

While the crystal order is spontaneously generated in this wave function, a complete characterization of the crystalline order requires knowledge of the phase of the order parameter $\Phi = S_A^z + S_B^z e^{i2\pi/3} + S_C^z e^{i4\pi/3} \equiv |\Phi| e^{i\theta}$, where $S_{A,B,C}^z$ refer to the total density on the A, B, C sublattices. Specifically the two candidate $\sqrt{3} \times \sqrt{3}$ crystal orders for this model have $\theta = 2n\pi/6$ with $n = 0, \dots, 5$, which corresponds to having a density order $(2m_z, -m_z, -m_z)$ on the three sublattices, and $\theta = (2n+1)\pi/6$ with $n = 0, \dots, 5$, which implies $(0, m_z, -m_z)$ order. Since the Jastrow factors are insensitive to the phase of Φ , they cannot select between these candidates. In order to find the optimal supersolid, we therefore include a factor $\mathcal{J}_\theta = \exp(h_\theta \cos 6\theta)$ in the wave function, with h_θ being a variational parameter. Optimizing this variational parameter, we find that $h_\theta > 0$ has the lowest energy indicating that the best supersolid state has $(2m_z, -m_z, -m_z)$ crystal order. As shown in Fig. 2(b) for $J_z = \infty$, the probability distribution $P(\theta)$, of the phase θ , shows sharp peaks at the expected angles at the optimal $h_\theta > 0$ [14], while the state with $h_\theta = 0$ is relatively featureless (the small peaks at $\theta = (2n+1)\pi/6$ appear to be a finite size artifact). Our results are consistent with earlier QMC simulation results [8, 10, 11] and recent variational calculations [12] in the quantum dimer model limit at $J_z = \infty$. Motivated by these re-

TABLE I: Exact diagonalization energy [16] versus variational energy of $|\Psi_V^{\text{AF-xy}}\rangle$ for a 6×6 system with $J_z \leq 1$.

J_z	0.0	0.5	0.9	1.0
VMC	-0.40950(7)	-0.46992(5)	-0.53075(5)	-0.54816(9)
ED	-0.410957	-0.475366	-0.541988	-0.560373

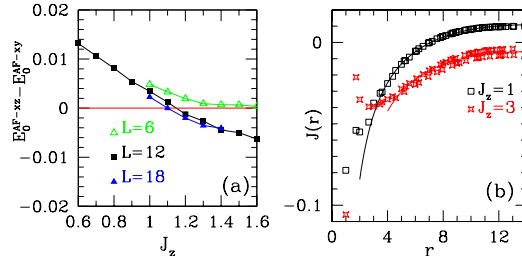


FIG. 3: (Color online) (a) Energy difference $\Delta E = E_0^{\text{AF-xz}} - E_0^{\text{AF-xy}}$ showing that $|\psi_V^{\text{AF-xz}}\rangle$ has lower energy for $J_z \gtrsim 1$. (b) Jastrow parameters versus distance for $J_z = 1$ ($|\psi_V^{\text{AF-xy}}\rangle$) and $J_z = 3$ ($|\psi_V^{\text{AF-xz}}\rangle$). Solid line depicts $1/r$ behavior. Curve for $J_z = 1$ has been shifted upward for clarity.

sults, we study the properties of $|\Psi_V^{\text{FM-xz}}\rangle$ which imposes the above supersolid order, and find that the optimized wave function of this type exhibits a small density deviation away from half-filling. Equivalently, the XXZ model has a spontaneous S^z magnetization in the supersolid.

$J_\perp > 0$, *Frustrated Case*. — For the frustrated model, the sign problem prevents controlled QMC simulations on large lattices. There have been some classical and spin wave analyses for large spin [15], and exact diagonalization (ED) studies on small systems [16] which do not address the issue of the thermodynamic limit for spin-1/2. The classical ground state with $J_z < 1$ has 120° magnetic ordering in the xy -plane. We therefore begin with the wavefunction $|\Psi_V^{\text{AF-xy}}\rangle$ as a variational candidate. With increasing J_z , the system becomes more strongly correlated, developing strong short range S^z correlations. Table I shows that the variational energy compares well with ED results [16] on a 6×6 lattice for $J_z \leq 1$.

From the density structure factor and probability distributions of the phase of Φ , defined earlier, we find that this wave function also displays a spontaneously ordered $\sqrt{3} \times \sqrt{3}$ supersolid, with staggered charge and superfluid orders, for $J_z \gtrsim 1.2$. The charge order is of the type $(2m_z, -m_z, -m_z)$ on the three sublattices, identical to what we found in the unfrustrated model, and m_z grows continuously beyond $J_z \approx 1.2$, whereas the superfluid order is of the type $(0, m_\perp, -m_\perp)$ on the 3 sublattices. Motivated by the proximity of this transition to the Heisenberg model, we compare the two states, $|\Psi_V^{\text{AF-xy}}\rangle$ and $|\Psi_V^{\text{AF-xz}}\rangle$, to see if the plane of the coplanar order rotates at this $SU(2)$ symmetric point. As shown in Fig. 3(a), the energy of $|\Psi_V^{\text{AF-xz}}\rangle$ is indeed lower for $J_z \gtrsim 1$. We find

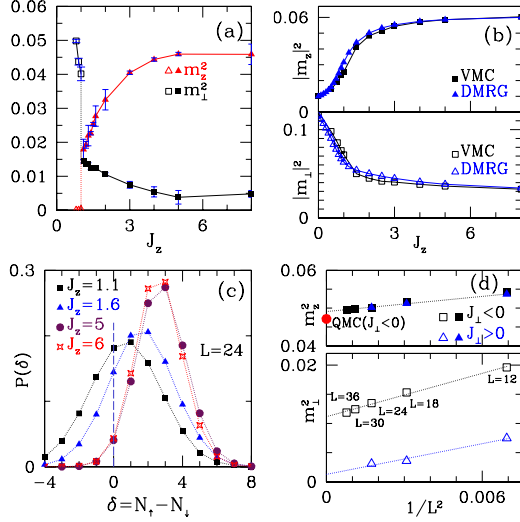


FIG. 4: (Color online) (a) Diagonal and off-diagonal order parameters extrapolated to the thermodynamic limit showing the order parameter discontinuity at $J_z \simeq 1$ and the coexistence of both orders for $J_z > 1$. (b) Order parameters for a 6×6 system compared with DMRG results from Ref.[7]. (c) Density distribution in $|\Psi_V^{\text{AF-xz}}\rangle$ showing nonzero magnetization with the onset of supersolid order. (d) Diagonal and off-diagonal order parameters in the limit $J_z = \infty$ showing good agreement of the extrapolated m_z^2 for $J_\perp > 0$ with QMC data on the unfrustrated model.

that the Jastrow factors in $|\Psi_V^{\text{AF-xy}}\rangle$ as well as $|\Psi_V^{\text{AF-xz}}\rangle$ exhibit a long range $1/r$ tail consistent with a linearly dispersing mode (see Fig. 3(b)).

Using the two different wave functions on the two sides of the Heisenberg point, we conclude that m_z and m_\perp are discontinuous at $J_z = 1$, and $|\Psi_V^{\text{AF-xz}}\rangle$ describes a supersolid state as seen from Fig. 4(a). For a 6×6 system, our results are in excellent agreement with DMRG calculations [7] (see Fig. 4(b)). The crystal order grows monotonically for $J_z > 1$, while m_\perp gets strongly suppressed. We find that $|\Psi_V^{\text{AF-xz}}\rangle$ exhibits a small spontaneous density deviation from half-filling, as shown in Fig. 4(c), which grows with J_z to a maximum value $\approx 0.05\%$.

$J_z = \infty$, the Quantum Dimer Limit. — At $J_z = \infty$, the Hilbert space of the XXZ model gets constrained to the minimally frustrated classical configurations of the triangular lattice Ising antiferromagnet [1]. Remarkably, although the ‘frustrated supersolid’ wave function $|\Psi_V^{\text{AF-xz}}\rangle$ describes a very different state from the ‘unfrustrated supersolid’ $|\Psi_V^{\text{FM-x}}\rangle$, we find, upon projecting to the minimally frustrated Ising subspace, that the crystal order parameters of both states are nearly equal, and are in good agreement with the extrapolated QMC result for the unfrustrated case, as shown in Fig. 4(d). We also find that the energies of these two completely different states are fairly close, within 6% of each other. This is consistent with recently uncovered exact results [6, 7] at $J_z = \infty$

which show that the crystal order parameters and ground state energies should be equal for either sign of J_\perp . As seen from Fig. 4(d), m_\perp extrapolates to a small value for either sign of J_\perp , with $m_\perp(J_\perp = 1) \ll m_\perp(J_\perp = -1)$.

Summary. — In summary, we have used a variational approach to obtain the phase diagram of the frustrated and unfrustrated spin-1/2 XXZ models on the triangular lattice for large lattice sizes and arbitrary $J_z > 0$; these regimes are not accessible via other techniques. The phase diagram of the unfrustrated model is in good agreement with QMC data. The frustrated model exhibits a wide regime of supersolidity with no evidence of a spin liquid. Our results for $J_\perp < 0$ could be tested using polarized dipolar bosonic molecules in a triangular lattice by tuning the ratio J_\perp/J_z . For the frustrated model, proposed schemes to induce fictitious gauge fields [17] need to be adapted to produce a frustrated molecule hopping.

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